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Shortcuts to adiabaticity assisted by counterdiabatic Born–Oppenheimer dynamics

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Abstract

Shortcuts to adiabaticity (STA) provide control protocols to guide the dynamics of a quantum system through an adiabatic reference trajectory in an arbitrary prescheduled time. Designing STA proves challenging in complex quantum systems when the dynamics of the degrees of freedom span different time scales. We introduce counterdiabatic Born–Oppenheimer dynamics (CBOD) as a framework to design STA in systems with a large separation of energy scales. CBOD exploits the Born–Oppenheimer approximation to separate the Hamiltonian into effective fast and slow degrees of freedom and calculate the corresponding counterdiabatic drivings for each sub-system. We show the validity of the CBOD technique via an example of coupled harmonic oscillators, which can be solved exactly for comparison, and further apply it to a system of two-charged particles.

1. Introduction

Tailoring the nonadiabatic dynamics of quantum matter is an open problem at the frontiers of physics with important applications in emergent quantum technologies. Control protocols relying on adiabatic dynamics are natural to prescribe the evolution of a system along a reference adiabatic trajectory. While they are robust against uncontrolled errors in the experimental implementation, they are susceptible to decoherence. Driving protocols known as shortcuts to adiabaticity (STA) provide an alternative, by speeding up an adiabatic reference trajectory of a quantum system in a prescheduled amount of time [1].

STA have found broad applications in quantum mechanical systems of varying complexity. They can be used to guide the dynamics of systems with a discrete energy spectrum [2–7], as shown in the laboratory [8–11]. Similarly, STA can be used to control the degrees of freedom of continuous variables systems [1, 12–19] as demonstrated by the fast control of a trapped ion in phase space [20]. In the context of trapped ultracold atoms, early theoretical results indicated that STA could be applied to many-body systems [17, 21–23]. Ultrafast expansions and compressions of atomic clouds have by now been implemented in a wide variety of interaction regimes including thermal clouds [24], Bose–Einstein condensates well described by mean field theory [25, 26], tightly confined quasi-one-dimensional atomic clouds with phase fluctuations [27], and a unitary Fermi gas as a paradigmatic instance of a strongly-coupled quantum fluid [28, 29]. In addition, theoretical studies have shown that STA can be used to guide the evolution of many-body quantum systems that exhibit quantum critical behavior [30, 31]. In this context, STA can be used to suppress excitation formation across a phase transition [32]. Implementing STA may require modifying the systems Hamiltonian with nonlocal interactions including high order terms [30, 33]. However, the required controls may be simplified or absorbed into the form of the original system Hamiltonian [34–37]. Further efforts to control the dynamics of many-body systems have been put forward relying on integrability (e.g. the existence of Lax pairs) [38] or variational methods [39]. Despite this surge of progress, applications of STA remain mostly confined to systems with few degrees of freedom or the control of certain collective modes in many-body quantum systems.

Designing STA requires the ability to control and describe the time-evolution of a system, an ubiquitous challenge across a variety of fields when dealing with complex quantum systems. Among them, a prominent instance occurs in quantum chemistry, in the study of quantum systems with degrees of freedom spanning different time and energy scales [40]. When the separation of scales is sufficiently large, it is possible to decouple the dynamics via the Born–Oppenheimer approximation (BOA) [41]. Born and Oppenheimer considered the description of a molecule and harnessed the separation of energy scales between the electronic and nuclear rotational and vibrational motions to simplify the description. As the electronic mass is much smaller than that of the atomic nuclei, the motion of the corresponding degrees of freedom occurs on vastly different time scales. When the mass ratio is large enough, the electrons move in an effectively static configuration of the nuclei. Further, this separation leads to the evolution of the nuclear component in the presence of a potential set by the energy of the electronic motion. When the assumptions of the approximation are relaxed, the nuclear motion is subject to a Berry vector potential due to the electronic motion [42–46]. Understanding the BOA and its limits has proved particularly fruitful in the field of spectroscopy [47, 48], the study of molecular dynamics, and in computational models [49–58]. There has also been recent advances in the quantum simulation of molecular dynamics, with the recent proposal and experimental implementation of vibrational spectroscopy with trapped ions via boson sampling [59–61].

In this paper, we introduce Counterdiabatic Born–Oppenheimer dynamics (CBOD) as an efficient technique for the fast control of complex systems that are well described by the BOA. To this end, we first provide a brief summary of the BOA and the engineering of STA by counterdiabatic driving (CD) in sections 2 and 3, respectively. We then present CBOD in section 4 and demonstrate its validity with a paradigmatic example of coupled harmonic oscillators of unequal mass, in section 5. We end by considering an example of a trapped particle and free particle interacting via a Coulomb-like term in section 6.

2. Born–Oppenheimer method

In order to fix the notation, we will briefly discuss the BOA that will be at the core of the CBOD technique. Throughout this work, we will consider two-body systems. However, the approach can be readily generalized to N-body systems with two sub-sets of slow (heavy) and fast (light) particles, that we indicate with the labels S and F, respectively. We will make the assumption that $m_S \gg m_F$. In this section, we will introduce both the conventional BOA as well as the relaxed BOA, whereby, the fast degrees of freedom give rise to a Berry vector potential for the slow variables.

2.1. Conventional BOA

Consider a Hamiltonian of the form

$$\hat{H} = \frac{\hat{\mathbf{p}}_S^2}{2m_S} + \frac{\hat{\mathbf{p}}_F^2}{2m_F} + V(\hat{\mathbf{x}}_S, \hat{\mathbf{x}}_F), \tag{1}$$

where $\hat{\mathbf{p}}_i = -\mathrm{i}\hbar\nabla_i$ $(i = S, F)$ denotes the momentum operator and $V(\hat{\mathbf{x}}_S, \hat{\mathbf{x}}_F)$ is a global potential term. The latter can generally be decomposed as

$$V(\hat{\mathbf{x}}_S, \hat{\mathbf{x}}_F) = V_S(\hat{\mathbf{x}}_S) + V_F(\hat{\mathbf{x}}_F) + V_I(\hat{\mathbf{x}}_S, \hat{\mathbf{x}}_F), \tag{2}$$

with the first two terms acting exclusively on the slow and fast coordinates, respectively, and an interaction term, which is not separable in the coordinate representation in terms of $\{x_S, x_F\}$. The general form given by this Hamiltonian includes the usual molecular Hamiltonian for electronic and nuclear dynamics, frequently used in quantum chemistry [41, 47, 62].

We wish to obtain the solutions to the Schrödinger equation

$$\left[\frac{\hat{\mathbf{p}}_S^2}{2m_S} + \frac{\hat{\mathbf{p}}_F^2}{2m_F} + V(\hat{\mathbf{x}}_S, \hat{\mathbf{x}}_F)\right]\Psi = E\,\Psi. \tag{3}$$

Given the difference in mass ($m_S \gg m_F$), the BOA suppresses the kinetic energy term of the slow variables [63] to obtain a reduced Hamiltonian for the fast ones. As $\hat{\mathbf{x}}_S$ commutes with this reduced Hamiltonian, we can simultaneously obtain the solutions of the reduced and full sub-systems. The reduced Hamiltonian governs the Schrödinger equation of the fast sub-system

$$\left[\frac{\hat{\mathbf{p}}_F^2}{2m_F} + V(\mathbf{x}_S, \hat{\mathbf{x}}_F)\right]\phi_n(\mathbf{x}_F; \mathbf{x}_S) = \varepsilon_n(\mathbf{x}_S)\phi_n(\mathbf{x}_F; \mathbf{x}_S). \tag{4}$$

The slow coordinates $\mathbf{x}_S$ can be regarded as a parameter on which the reduced system eigenvalues and eigenvectors depend. The solutions to the reduced Schrödinger equation form a complete set, in terms of which

the full solution to the complete Schrödinger equation, equation (3), can be written as

$$\Psi = \sum_n \phi_n(\mathbf{x}_F; \mathbf{x}_S)\psi_n(\mathbf{x}_S), \tag{5}$$

where n runs over the eigenstates of the reduced Hamiltonian. We will assume in this work that the fast sub-system is in a single eigenstate n, avoiding the need for the summation in equation (5).

Using the product expansion of the wave function, equation (5), and the reduced Schrödinger equation, equation (4), the full Schrödinger equation reads

$$\left[\frac{\hat{\mathbf{p}}_S^2}{2m_S} + \varepsilon_n(\hat{\mathbf{x}}_S)\right]\phi(\mathbf{x}_F; \mathbf{x}_S)\psi(\mathbf{x}_S) = E\phi(\mathbf{x}_F; \mathbf{x}_S)\psi(\mathbf{x}_S). \tag{6}$$

In the conventional BOA the derivatives of the fast sub-system wave function, $\phi(\mathbf{x}_F; \mathbf{x}_S)$, with respect to $\mathbf{x}_S$ are neglected in the above equation, i.e.,

$$\frac{\hat{\mathbf{p}}_S^2}{2m_S}\phi(\mathbf{x}_F; \mathbf{x}_S)\psi(\mathbf{x}_S) \approx \phi(\mathbf{x}_F; \mathbf{x}_S)\frac{\hat{\mathbf{p}}_S^2}{2m_S}\psi(\mathbf{x}_S). \tag{7}$$

Integrating out the fast degrees of freedom is then straightforward and leads to a slow sub-system Schrödinger equation in the final form

$$\left[\frac{\hat{\mathbf{p}}_S^2}{2m_S} + \varepsilon_n(\hat{\mathbf{x}}_S)\right]\psi(\mathbf{x}_S) = E\ \psi(\mathbf{x}_S). \tag{8}$$

Note, E gives the full energy of the system while the full approximate wave function is given by equation (5).

The conventional BOA involves truly two approximations: (1) the energy scales of the system are vastly different allowing for the suppression of one of the kinetic energies to obtain the reduced Hamiltonian and (2) corrections due to the elimination of derivatives in $\mathbf{x}_S$ of the reduced wave function are small. These corrections are referred to as *diagonal corrections* and they are usually negligible in comparison to the energy scale of the fast sub-system [47]. The form of these corrections and their calculation is a vibrant area of research in its own right [64–71]. We have added another approximation to the conventional approach, that the fast sub-system evolves adiabatically, this was invoked when the sum over the fast sub-system states was neglected. This is a common approximation when using the BOA to describe time-evolution [47, 72], as the fast sub-system is assumed to quickly relax to its ground state in the time-scale of the slow motion. Note, that when we combine the BOA with CD, we will assume the fast sub-system either evolves adiabatically or, more importantly for our approach, that the fast sub-system is driven such that adiabaticity is enforced; in either case, the adiabatic approximation is met.

2.2. Relaxed BOA

The approximation involving the elimination of the derivatives with respect to $\mathbf{x}_S$ made in the conventional BOA can be relaxed [44, 45]. Generally, the neglected diagonal term can couple arbitrary eigenfunctions of the fast degrees of freedom. A relaxed BOA consists of keeping the resulting cross-terms of the $\mathbf{x}_S$ derivative while neglecting transitions between these different eigenstates. This leads to the appearance of a Berry connection between the two sub-systems in the full Schrödinger equation, which plays a role analogous to the vector potential in the quantum mechanics of a charged particle in an electromagnetic field [44, 45, 73].

Starting from the Schrödinger equation (6), our goal is to obtain a Schrödinger equation which is solely dependent on the slow degree of freedom, without invoking the previous approximation that disregards the derivatives of the momentum operator. To remove the fast degree of freedom we multiply equation (6) from the left by $\phi(\mathbf{x}_F; \mathbf{x}_S)^\dagger$ and integrate over $\mathbf{x}_F$ to obtain

$$\int d\mathbf{x}_F \phi(\mathbf{x}_F; \mathbf{x}_S)^\dagger \left[\frac{\hat{\mathbf{p}}_S^2}{2m_S} + \varepsilon_n(\hat{\mathbf{x}}_S)\right]\phi(\mathbf{x}_F; \mathbf{x}_S)\psi(\mathbf{x}_S) = \int d\mathbf{x}_F \phi(\mathbf{x}_F; \mathbf{x}_S)^\dagger E\phi(\mathbf{x}_F; \mathbf{x}_S)\psi(\mathbf{x}_S). \tag{9}$$

There is only one non-trivial integral in the above Schrödinger equation, which is,

$$\int d\mathbf{x}_F \phi(\mathbf{x}_F; \mathbf{x}_S)^\dagger \frac{\hat{\mathbf{p}}_S^2}{2m_S}\phi(\mathbf{x}_F; \mathbf{x}_S)\psi(\mathbf{x}_S). \tag{10}$$

It is an algebraic exercise [63] to obtain the terms arising from this integral, which can be written in terms of a vector and a scalar potential in the slow sub-system Schrödinger equation

$$\left[-\frac{\hbar^2}{2m_S}(\nabla_{\mathbf{x}_S}-\mathrm{i}A(\mathbf{x}_S))^2+\frac{\hbar^2}{2m_S}g(\mathbf{x}_S)+\varepsilon_n(\hat{\mathbf{x}}_S)\right]\psi(\mathbf{x}_S)=E\,\psi(\mathbf{x}_S) \tag{11}$$

with

$$\begin{aligned}\mathcal{A}(\mathbf{x}_S)&=\mathrm{i}\int \mathrm{d}\mathbf{x}_F\phi(\mathbf{x}_F;\,\mathbf{x}_S)^\dagger\nabla_{\mathbf{x}_S}\phi(\mathbf{x}_F;\,\mathbf{x}_S)\\&=\mathrm{i}\langle\phi|\nabla_{\mathbf{x}_S}\phi\rangle,\end{aligned} \tag{12}$$

$$\begin{aligned}g(\mathbf{x}_S)&=\int \mathrm{d}\mathbf{x}_F[\nabla_{\mathbf{x}_S}\phi(\mathbf{x}_F;\,\mathbf{x}_S)^\dagger]\nabla_{\mathbf{x}_S}\phi(\mathbf{x}_F;\,\mathbf{x}_S)+\left[\int \mathrm{d}\mathbf{x}_F\phi(\mathbf{x}_F;\,\mathbf{x}_S)^\dagger\nabla_{\mathbf{x}_S}\phi(\mathbf{x}_F;\,\mathbf{x}_S)\right]^2\\&=\langle\nabla_{\mathbf{x}_S}\phi|\nabla_{\mathbf{x}_S}\phi\rangle-\langle\nabla_{\mathbf{x}_S}\phi|\phi\rangle\langle\phi|\nabla_{\mathbf{x}_S}\phi\rangle.\end{aligned} \tag{13}$$

The vector potential $\mathcal{A}(\mathbf{x}_S)$ is the familiar Berry connection. The scalar potential $\varepsilon_n(\hat{\mathbf{x}}_S)$ is local and is dictated by the fast variables. In addition, there is a contribution to the scalar potential experienced by the slow degrees of freedom that is given by $g(\mathbf{x}_S)$, which is the trace of the quantum geometric tensor [74] associated with the change of the eigenstates $|\phi\rangle$ with respect to the slow coordinates $\mathbf{x}_S$, treated as a parameter.

3. Counterdiabatic driving

Among the variety of techniques available to engineer STA, CD stands out as a universal approach. It relies on the use of auxiliary counterdiabatic fields to guide the evolution of the quantum system of interest through an adiabatic reference trajectory. CD was developed in the context of molecular dynamics by Demirplak and Rice [2, 3, 75], as an alternative to strictly adiabatic population transfers between molecular states; see also the independent and closely related work by Berry [4]. CD and related protocols have been recently implemented in a variety of platforms for quantum technologies including trapped ions [20], nitrogen-vacancy centres in diamond [9, 11], ultracold atoms in optical lattices [8] and as a method to speed up stimulated Raman adiabatic passage in ultracold gases [10]. It has become a popular technique to control and engineer the nonadiabatic evolution of quantum systems while enforcing the following of adiabatic trajectories [2–4, 23, 39, 75].

CD relies on the spectral properties, eigenstates and energies, of the driven Hamiltonian of interest

$$\hat{H}_0(t)|n(t)\rangle=\varepsilon_n(t)|n(t)\rangle. \tag{14}$$

According to the adiabatic approximation, the state of a system prepared in an eigenstate $|n(0)\rangle$ at $t=0$ evolves under a slowly-varying $\hat{H}_0(t)$ into

$$|\psi_n^{\mathrm{ad}}(t)\rangle=\exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\varepsilon_n(t')-\int_0^t \mathrm{d}t'\langle n(t')|\partial_{t'}n(t')\rangle\right]|n(t)\rangle, \tag{15}$$

which includes the dynamical phase as well as the geometric phase associated with the Berry connection $\mathrm{i}\langle n(t')|\partial_{t'}n(t')\rangle$.

A STA protocol assisted by CD can be designed by identifying a modified driven Hamiltonian $\hat{H}(t)$ such that the adiabatic evolution (15) becomes the exact solution of the corresponding time-dependent Schrödinger equation

$$\hat{H}(t)|\psi_n^{\mathrm{ad}}(t)\rangle=\mathrm{i}\hbar\,\partial_t|\psi_n^{\mathrm{ad}}(t)\rangle. \tag{16}$$

Hence, no matter how fast the system is driven, the evolution is described by the adiabatic trajectory (15), i.e., without the requirement of slow driving. The corresponding time-evolution operator also fulfills (16), which allows the identification of the modified driven Hamiltonian as the generator of evolution

$$\hat{H}(t)=\mathrm{i}\hbar\,[\partial_t\hat{U}(t)]\,\hat{U}^\dagger(t). \tag{17}$$

Making use of the following form of the time-evolution operator

$$\hat{U}(t)=\sum_n|\psi_n^{\mathrm{ad}}(t)\rangle\langle n(0)|, \tag{18}$$

the modified driven Hamiltonian is found by explicit computation [2, 4]

$$\hat{H}(t)=\sum_n\varepsilon_n|n\rangle\langle n|+\hat{H}_1(t), \tag{19}$$

where we have defined

$$\hat{H}_1(t) = \mathrm{i}\hbar \sum_n (|\partial_t n\rangle \langle n| - \langle n|\partial_t n\rangle |n\rangle \langle n|). \tag{20}$$

The first term in (19) is recognized as the spectral decomposition of the original system Hamiltonian $\hat{H}_0(t)$. The second term, $\hat{H}_1$, is the auxiliary CD term required so that the adiabatic trajectory $|\psi_n^{\mathrm{ad}}(t)\rangle$ in equation (15) becomes an exact solution of (16), that is the Schrödinger equation for the full driving Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$.

When the energy spectrum of $\hat{H}_0$ is non-degenerate, the additional CD term can be recasted using the differential of the time-independent Schrödinger equation of the original system Hamiltonian [4], $\hat{H}_0(t)$,

$$\langle m(t)|\partial_t n(t)\rangle = \frac{\langle m(t)|\partial_t \hat{H}_0(t)|n(t)\rangle}{\varepsilon_n(t) - \varepsilon_m(t)}, \tag{21}$$

which yields the following alternative expression for the auxiliary CD term

$$\hat{H}_1(t) = \mathrm{i}\hbar \sum_{m\neq n} \sum_n \frac{\hat{P}_m(t)\partial_t \hat{H}_0(t)\hat{P}_n(t)}{\varepsilon_n(t) - \varepsilon_m(t)}, \tag{22}$$

in terms of the projector $\hat{P}_m(t) = |m(t)\rangle \langle m(t)|$.

4. Counterdiabatic Born–Oppenheimer Dynamics (CBOD)

The Born–Oppenheimer method and the theory of CD can be exploited jointly to engineer the fast nonadiabatic control of complex systems, as we next discuss. The CDs for the slow and fast sub-systems can be obtained via the BOA, either via the conventional or relaxed variants. These auxiliary control terms can then be used to drive the (exact) system Hamiltonian, a technique we shall term as CBOD.

4.1. CD with the conventional BOA

We first consider the conventional BOA, according to which the fast and slow sub-system Hamiltonians are

$$\hat{H}_F(\hat{\mathbf{x}}_F, t; \mathbf{x}_S) = \frac{\hat{\mathbf{p}}_F^2}{2m_F} + V(\mathbf{x}_S, \hat{\mathbf{x}}_F), \tag{23}$$

$$\hat{H}_S(\hat{\mathbf{x}}_S, t) = \frac{\hat{\mathbf{p}}_S^2}{2m_S} + \varepsilon_n(\hat{\mathbf{x}}_S). \tag{24}$$

The required CD terms can be found via the general expression equation (20) and for the slow and fast sub-systems read, respectively,

$$\hat{H}_{F,1}(t) = \mathrm{i}\hbar\,(|\partial_t \phi\rangle \langle \phi| - \langle \phi|\partial_t \phi\rangle |\phi\rangle \langle \phi|), \tag{25}$$

$$\hat{H}_{S,1}(t) = \mathrm{i}\hbar\,(|\partial_t \psi\rangle \langle \psi| - \langle \psi|\partial_t \psi\rangle |\psi\rangle \langle \psi|). \tag{26}$$

By contrast, the CD term for the full system is

$$\hat{H}_{\mathrm{Full},1}(t) = \mathrm{i}\hbar\,(|\partial_t \Psi\rangle \langle \Psi| - \langle \Psi|\partial_t \Psi\rangle |\Psi\rangle \langle \Psi|). \tag{27}$$

The full form can be rewritten, exploiting the tensor product structure of the full wave function $|\Psi\rangle = |\phi\rangle \otimes |\psi\rangle$ (i.e. separable in the BOA). We note that while this separable form is natural in the BOA, it can be invoked generally [76, 77]. Substituting in the factored form of the full wave function, the full CD can be written as

$$\begin{aligned}\hat{H}_{\mathrm{Full},1}(t) &= \mathrm{i}\hbar(|\partial_t \phi\rangle\langle\phi| \otimes |\psi\rangle\langle\psi| + |\phi\rangle\langle\phi| \otimes |\partial_t \psi\rangle\langle\psi| - \langle\phi|\partial_t\phi\rangle \otimes |\psi\rangle\langle\psi| - |\phi\rangle\langle\phi| \otimes \langle\psi|\partial_t\psi\rangle) \\ &\equiv \hat{H}_{F,1}(t) \otimes |\psi\rangle\langle\psi| + |\phi\rangle\langle\phi| \otimes \hat{H}_{S,1}(t).\end{aligned} \tag{28}$$

Therefore, the CBOD technique simplifies the global CD control by driving the two sub-systems separately, this is, by using the auxiliary control terms (25) and (26) as opposed to (27).

We can gain further insight into the CBOD terms by assuming the spectra of $\hat{H}_S$ and $\hat{H}_F$ to be non-degenerate, as this allows the recasting of the CD control terms into the form of equation (22),

$$\hat{H}_{F,1} = \mathrm{i}\hbar \sum_{m\neq n} \sum_n \frac{|\phi_m\rangle \langle \phi_m|\partial_t V(\mathbf{x}_S, \hat{\mathbf{x}}_F)|\phi_n\rangle \langle \phi_n|}{\varepsilon_n(\mathbf{x}_S) - \varepsilon_m(\mathbf{x}_S)}, \tag{29}$$

$$\hat{H}_{S,1} = \mathrm{i}\hbar \sum_{m\neq n} \sum_n \frac{|\psi_m\rangle \langle \psi_m|\partial_t \varepsilon_n(\hat{\mathbf{x}}_S)|\psi_n\rangle \langle \psi_n|}{E_n - E_m}. \tag{30}$$

Note, that in the fast control $\hat{H}_{F,1}$, $\mathbf{x}_S$ is treated as a parameter, which is the case of the reduced Hamiltonian in equation (4) in the BOA.

As customary in STA assisted by CD, the required auxiliary terms are off-diagonal in state space. However, it is useful to focus on the dependencies on $\mathbf{x}_S$ and $\mathbf{x}_F$. We wish to compare the CBOD terms with the exact CD term without resorting to the BOA. Assuming the system is exactly solvable the CD is

$$\hat{H}_{\text{exact},1} = \mathrm{i}\hbar \sum_{m\neq n}\sum_{n} \frac{|\chi_m\rangle\langle\chi_m|\partial_t V(\hat{\mathbf{x}}_S, \hat{\mathbf{x}}_F)|\chi_n\rangle\langle\chi_n|}{\epsilon_n - \epsilon_m}, \tag{31}$$

with $\hat{H}_0|\chi_n\rangle = \epsilon_n|\chi_n\rangle$, $|\chi\rangle$ the exact eigenstates and ϵ_n the exact eigenvalues. Due to the interactions between slow and fast degrees of freedom, which are not separable in the $\{\mathbf{x}_S, \mathbf{x}_F\}$ space, the operator $\hat{H}_{\text{exact},1}$ can be complicated to implement, as it involves a generally complex coupling between the two sub-spaces (or two particles).

Therefore, CBOD provides a computational advantage over the exact STA approach. Indeed, it circumvents the need to deal with the full spectra, proceeding, instead, in two-subsequent steps; treating first the fast degrees of freedom and then the slow ones. CBOD thus benefits from the dimensional reduction of the problem to engineer the CD term for the fast sub-system driving, equation (29).

In addition, CBOD may simplify the required drivings by potentially removing or reducing the coupling between the two sub-spaces. In such a case, CBOD controls will be simpler to implement than the exact CD terms. For the slow sub-system, equation (30), the off-diagonal terms are coupled via the time derivative of the energy for the fast sub-system. This is the potential surface which the slow sub-system experiences due to the fast sub-system, and it is of no surprise that to enforce adiabatic evolution it is required to drive off-diagonal terms with this as the scaling. The coordinate dependence of slow sub-system CD, equation (30) is simplified in comparison to the exact driving, equation (31), as the potential energy surfaces can only depend on $\mathbf{x}_S$. Therefore, the slow sub-system driving only requires operators which act on the slow sub-system space and will have no cross-terms between the two sub-spaces. Therefore, CBOD readily simplifies the required control term for the slow sub-system, without further approximations.

4.2. CD with the relaxed BOA

In what follows we derive the modified driving controls when the relaxed BOA is used, as discussed in section 2.2. The required CD terms for the fast and exact systems are the same as in equations (25) and (27); alternatively, by (29) and (31). The slow sub-system has a modified Hamiltonian resembling that of a particle in an electromagnetic field, see equation (11).

To obtain the CD under the assumption of no degeneracies in the spectra according to equation (22), we first need to obtain the time derivative of the Hamiltonian

$$\partial_t \hat{H}_S = \frac{\hbar^2}{2m_S}[2\mathrm{i}(\partial_t A)\nabla_{\mathbf{x}_S} + 2A(\partial_t A) + \mathrm{i}(\nabla_{\mathbf{x}_S}\partial_t A)] + \frac{\hbar^2}{2m_S}\partial_t g_n + \partial_t \varepsilon_n. \tag{32}$$

The latter admits the compact form

$$\partial_t \hat{H}_S(\mathbf{x}_S, t) = \frac{\mathrm{i}\hbar}{m_S}\{\dot{\mathcal{A}}_n(\hat{\mathbf{x}}_S, t), \nabla_{\mathbf{x}_S}\} + \mathcal{V}_n(\hat{\mathbf{x}}_S, t), \tag{33}$$

with the potential term given by

$$V_n(\hat{\mathbf{x}}_S, t) = \frac{\hbar^2}{m_S}\mathcal{A}_n(\hat{\mathbf{x}}_S, t)\dot{\mathcal{A}}_n(\hat{\mathbf{x}}_S, t) - \frac{\mathrm{i}\hbar^2}{2m_S}\nabla_{\hat{\mathbf{x}}_S}\dot{\mathcal{A}}_n(\hat{\mathbf{x}}_S, t) + \frac{\hbar^2}{2m_S}\partial_t g_n(\hat{\mathbf{x}}_S, t) + \partial_t \varepsilon_n(\hat{\mathbf{x}}_S, t), \tag{34}$$

where $\{\cdot,\cdot\}$ denotes the anti-commutator and $\dot{\mathcal{A}} \equiv \partial_t \mathcal{A}$. The slow sub-system CD is therefore given by

$$\hat{H}_{S,1} = \mathrm{i}\hbar \sum_{m\neq n}\sum_{n} \frac{1}{E_n - E_m}\left[\hat{P}_{m,S}\left(\frac{\mathrm{i}\hbar}{m_S}\{\dot{\mathcal{A}}_n(\hat{\mathbf{x}}_S, t), \nabla_{\mathbf{x}_S}\} + V_n(\hat{\mathbf{x}}_S, t)\right)\hat{P}_{n,S}\right], \tag{35}$$

where $\hat{P}_{m,S} = |m_S\rangle\langle m_S|$. As a result, even with the relaxed BOA, the slow sub-system CD term only depends on operators related to the slow coordinate $\mathbf{x}_S$.

4.3. Applicability of CBOD

CBOD, as an approximate technique, does not necessarily enforce the evolution of the system Hamiltonian to follow the adiabatic trajectory exactly. It resorts to the CD terms constructed via the BOA to drive the (exact) system, which includes couplings between slow and fast sub-systems beyond BOA. Said differently, CBOD is constructed to drive the fast and slow Hamiltonians of the BOA Hamiltonian (as opposed to the exact system Hamiltonian) exactly through the adiabatic manifold. We will assess the validity of CBOD using the fidelity between the resulting state and that of the exact adiabatic evolution after a modulation of the system Hamiltonian in a prescheduled time.

The implementation of the CBOD technique, in general, involves the following steps:

1. Check the validity of BOA, i.e., that there are two separated energy scales in the region of interest.
2. Derive the CDs using the BOA.
3. Apply these (approximate) control terms to guide the dynamics of the (exact) system Hamiltonian.

We will consider next an example discussing each step in detail and certify CBOD by comparing its performance to the exact CD evolution.

5. Coupled harmonic system

To illustrate CBOD, we next consider the engineering of STA to drive two coupled harmonic oscillators, that can represent, e.g., two atoms in a harmonic trap interacting via a spring-like term. This model has been previously used to assess the BOA [78], admits an exact solution [79–84] and is realizable in controllable quantum systems of ion traps [85–88]. It, therefore, constitutes a natural test-bed for CBOD.

Specifically, we consider the Hamiltonian

$$\hat{H}_0(t) = \frac{\hat{p}_S^2}{2m_S} + \frac{\hat{p}_F^2}{2m_F} + \frac{1}{2}k_S(t)\hat{x}_S^2 + \frac{1}{2}k_F(t)\hat{x}_F^2 + \frac{1}{2}k_I(t)(\hat{x}_S - \hat{x}_F)^2, \tag{36}$$

with continuous variables $\hat{x}_S$ and $\hat{x}_F$ in one spatial dimension. Alternatively, it can be rewritten as

$$\hat{H}_0(t) = \frac{\hat{p}_S^2}{2m_S} + \frac{\hat{p}_F^2}{2m_F} + \frac{1}{2}\kappa_S(t)\hat{x}_S^2 + \frac{1}{2}\kappa_F(t)\hat{x}_F^2 - k_I(t)\hat{x}_S\hat{x}_F, \tag{37}$$

with $\kappa_S = k_S + k_I$ and $\kappa_F = k_F + k_I$, which makes explicit the bilinear coupling. For the sake of generality, we first provide a derivation of the CDs for this system when all spring constants are time-dependent.

The spectral properties can be studied by diagonalizing the system in terms of two independent harmonic oscillators, the normal modes. We denote by $\hat{y}_i$, $\hat{p}_i$, and $\kappa_i\,(i = 1, 2)$ the corresponding normal-mode coordinates, conjugate momentum and spring constants, for which explicit expressions are derived in the appendix. In terms of them, the system Hamiltonian can be simply written as

$$\hat{H}_0(t) = \frac{\hat{p}_1^2}{2\mu} + \frac{\hat{p}_2^2}{2\mu} + \frac{1}{2}\kappa_1(t)\hat{y}_1^2 + \frac{1}{2}\kappa_2(t)\hat{y}_2^2. \tag{38}$$

The BOA leads to an approximation of the system Hamiltonian $\hat{H}_0$ also in terms of two independent harmonic oscillators, whose eigenstates under the conventional and relaxed BOA coincide, as the Berry connection identically vanishes and the quantum geometric tensor reduces to a time-dependent constant; see the appendix for further details. Note, that in order for the slow sub-system of the BOA Hamiltonian to have a real harmonic frequency it is required that $\kappa_S(t)\kappa_F(t) > k_I(t)^2$.

Knowledge of the exact and BOA eigenfunctions allows us to establish the validity of the BOA whenever $m_F/m_S \ll 1$. To this end, we consider the fidelity between an exact eigenstate of the two coupled harmonic oscillators Ψ_{exact} and the corresponding BOA Ψ_{BOA}

$$F = |\langle \Psi_{\text{Exact}} | \Psi_{\text{BOA}} \rangle|^2. \tag{39}$$

The Born–Oppenheimer method provides a good approximation for the coupled harmonic oscillator problem for a small mass ratio m_F/m_S, see figure 1. As the trapping frequency of any of the two sub-systems—slow or fast particles—is increased, the accuracy of the BOA increases, as shown in figures 1(a)–(b). This is consistent with the fact that the energy scale separation between the two sub-systems is increased for a given mass ratio as the sub-system spring constants are made larger, making the two sub-systems more decoupled. By contrast, when decreasing the interaction strength, see figure 1(c), the state Ψ_{BOA} approaches Ψ_{Exact} as quantified by the higher values of the fidelity. Naturally, the coupling between both sub-systems increases with the interaction spring constant, leading to a breakdown of the BOA at large values of k_I.

We next derive and compare the auxiliary control terms required to enforce adiabaticity in an arbitrary prescheduled time using the exact CD and CBOD.

5.1. Exact CD

The exact solution of the coupled system (36) can be written in terms of the two independent harmonic oscillators, the normal modes, described by Hamiltonian (38). Knowledge of the CD term for a single harmonic oscillator [23, 89] readily yields the exact CD term for the coupled system

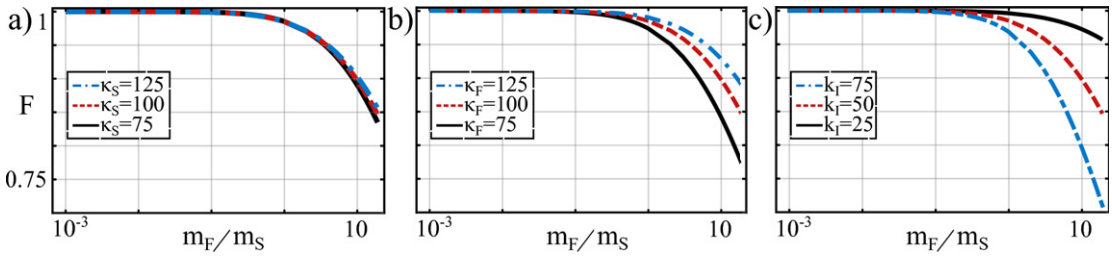

Figure 1. Ground state fidelity between the exact and BOA wave functions. Fidelity between the exact ground state wave function of two coupled harmonic oscillators and the corresponding BOA wave function, as a function of the mass ratio in a log-scale. (a) Increasing the slow spring constant, enhances the accuracy of BOA ($\kappa_F = 100, k_I = 50$). (b) Similarly, increasing the fast spring constant increases the fidelity ($\kappa_S = 100, k_I = 50$). (c) As the coupling between the slow and fast sub-systems is enhanced by increasing the interaction spring constant, the BOA begins to break down (with $\kappa_S = 100$ and $\kappa_F = 100$).

$$\hat{H}_1(t) = -\frac{\dot{\omega}_1(t)}{4\omega_1(t)}\{\hat{y}_1, \hat{p}_1\} - \frac{\dot{\omega}_2(t)}{4\omega_2(t)}\{\hat{y}_2, \hat{p}_2\}, \tag{40}$$

as the sum of the generators of the squeezing operator for each normal mode. As such, they are spatially non-local due to the momentum dependence. Alternative controls can be obtained by means of the unitary transformation

$$\mathcal{U} = \exp\left(-\frac{\mathrm{i}\mu\dot{\omega}_1(t)}{4\hbar\omega_1(t)}\hat{y}_1^2\right)\exp\left(-\frac{\mathrm{i}\mu\dot{\omega}_2(t)}{4\hbar\omega_2(t)}\hat{y}_2^2\right), \tag{41}$$

which acts on the position and momentum operators in the Hamiltonian as

$$\begin{aligned}
\hat{y}_{1,2} &\to U\hat{y}_{1,2}U^\dagger = \hat{y}_{1,2},\\
\hat{p}_{1,2} &\to U\hat{p}_{1,2}U^\dagger = \hat{p}_{1,2} + \frac{1}{2}\mu\frac{\dot{\omega}_{1,2}(t)}{\omega_{1,2}(t)}\hat{y}_{1,2},\\
\hat{p}_{1,2}^2 &\to U\hat{p}_{1,2}^2U^\dagger = \hat{p}_{1,2}^2 + \frac{\dot{\omega}_{1,2}(t)\mu}{2\omega_{1,2}(t)}\{\hat{y}_{1,2}, \hat{p}_{1,2}\} + \frac{\mu^2\dot{\omega}_{1,2}(t)^2}{4\omega_{1,2}(t)^2}\hat{y}_{1,2}^2.
\end{aligned} \tag{42}$$

Given that $\partial_t\mathcal{U}^\dagger \neq 0$ the full driving Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$ is transformed according to

$$\hat{H} \to \hat{H}_T = \mathcal{U}\hat{H}\mathcal{U}^\dagger - \mathrm{i}\hbar\,\mathcal{U}\partial_t\mathcal{U}^\dagger. \tag{43}$$

while the original wave function Ψ is mapped to

$$\Psi \to \Psi_T = \mathcal{U}\Psi. \tag{44}$$

Making use of (42), it is found that the transformed Hamiltonian $\hat{H}_T$, unitarily equivalent to $\hat{H}$, takes the form

$$\hat{H}_T(t) = \frac{\hat{p}_1^2}{2\mu} + \frac{\hat{p}_2^2}{2\mu} + \frac{1}{2}\mu\omega_{T,1}(t)^2\hat{y}_1^2 + \frac{1}{2}\mu\omega_{T,2}(t)^2\hat{y}_2^2, \tag{45}$$

with the corresponding frequencies being

$$\omega_{T,\{1,2\}}(t)^2 = \omega_{1,2}(t)^2 - \frac{3\dot{\omega}_{1,2}(t)^2}{4\omega_{1,2}(t)^2} + \frac{\ddot{\omega}_{1,2}(t)}{2\omega_{1,2}(t)}. \tag{46}$$

Therefore, the exact CD of coupled harmonic oscillators can be implemented by a modification of the normal mode frequency of the original system Hamiltonian $\hat{H}_0$. However, this modification will require independent control of the slow, fast and interaction spring constants.

5.2. CBOD

Within the BOA the Hamiltonians of the slow and fast sub-systems are that of two harmonic oscillators, and the corresponding CBOD terms are given by

$$\hat{H}_{F,1}(t) = -\frac{\dot{\omega}_F(t)}{4\omega_F(t)}\{\hat{x}_T, \hat{p}_T\}, \tag{47}$$

$$\hat{H}_{S,1}(t) = -\frac{\dot{\omega}_S(t)}{4\omega_S(t)}\{\hat{x}_S, \hat{p}_S\}, \tag{48}$$

where $\hat{x}_T = \left(\hat{x}_F - \frac{k_I(t)}{\kappa_F(t)}x_S\right)$ and $\hat{p}_T = \hat{p}_F$ is the corresponding conjugate momentum operator, see the appendix. For the coupled harmonic oscillators the CBOD auxiliary controls under the conventional and relaxed BOA are equivalent, as the wave functions coincide. We will consider a case in which the fast sub-system is also driven to

enforce adiabaticity by CBOD. However, within the BOA the fast sub-system is usually assumed to evolve adiabatically and, in that case, the control $\hat{H}_{F,1}$ would not be required. The driving Hamiltonian with the CBOD control terms reads

$$\hat{H}(t)=\frac{\hat{p}_S^2}{2m_S}+\frac{\hat{p}_F^2}{2m_F}+\frac{1}{2}\kappa_S(t)\hat{x}_S^2+\frac{1}{2}\kappa_F(t)\hat{x}_F^2-k_I(t)\hat{x}_S\hat{x}_F-\frac{\dot{\omega}_S}{4\omega_S}\{\hat{x}_S,\,\hat{p}_S\}-\frac{\dot{\omega}_F}{4\omega_F}\{\hat{x}_T,\,\hat{p}_F\}. \tag{49}$$

The evolution under this Hamiltonian is not necessarily adiabatic with respect to the exact $\hat{H}_0$ eigenbasis, as the CBOD auxiliary terms are approximate. As a result, an STA designed by CBOD cannot be arbitrarily fast. The direct exact solution of the Schrödinger equation with this Hamiltonian is hindered by the term $\hat{x}_S\hat{p}_F$ resulting from the last anti-commutator. However, this term can be absorbed into the fast momentum. Dropping the time dependence for simplicity, one finds

$$\begin{aligned}\frac{\hat{p}_F^2}{2m_F}+\frac{\dot{\omega}_F k_I}{2\omega_F\kappa_F}\hat{x}_S\hat{p}_F&=\frac{1}{2m_F}\left(\hat{p}_F+m_F\frac{\dot{\omega}_F k_I}{2\omega_F\kappa_F}\hat{x}_S\right)^2-m_F\frac{\dot{\omega}_F^2k_I^2}{8\omega_F^2\kappa_F^2}\hat{x}_S^2\\&\approx\frac{\hat{p}_F^2}{2m_F}-m_F\frac{\dot{\omega}_F^2k_I^2}{8\omega_F^2\kappa_F^2}\hat{x}_S^2,\end{aligned} \tag{50}$$

where in the final line we have made an approximation consistent with the BOA, that the fast sub-system momentum will dominate over the additional momentum term which is a function of the slow sub-system coordinate. The driving Hamiltonian takes then the form

$$\hat{H}(t)=\frac{\hat{p}_S^2}{2m_S}+\frac{\hat{p}_F^2}{2m_F}+\frac{1}{2}\left(\kappa_S(t)-m_F\frac{\dot{\omega}_F^2k_I^2}{4\omega_F^2\kappa_F^2}\right)\hat{x}_S^2+\frac{1}{2}\kappa_F(t)\hat{x}_F^2-k_I(t)\hat{x}_S\hat{x}_F-\frac{\dot{\omega}_S}{4\omega_S}\{\hat{x}_S,\,\hat{p}_S\}-\frac{\dot{\omega}_F}{4\omega_F}\{\hat{x}_F,\,\hat{p}_F\}. \tag{51}$$

In a similar manner to the previous scenario, we can use the unitary transformation of

$$\mathcal{U}=\exp\left[-\mathrm{i}\left(\frac{m_S\dot{\omega}_S(t)}{4\hbar\omega_S(t)}x_S^2+\frac{m_F\dot{\omega}_F(t)}{4\hbar\omega_F(t)}x_F^2\right)\right] \tag{52}$$

to obtain the unitarily equivalent Hamiltonian

$$\hat{H}(t)=\frac{\hat{p}_S^2}{2m_S}+\frac{\hat{p}_F^2}{2m_F}+\frac{1}{2}\gamma_S(t)\hat{x}_S^2+\frac{1}{2}\gamma_F(t)\hat{x}_F^2-k_I(t)\hat{x}_S\hat{x}_F \tag{53}$$

which is that of two oscillators with bilinear coupling, i.e., the original system Hamiltonian (51), with modified spring constants

$$\gamma_S=\kappa_S-\frac{3m_S\dot{\omega}_S^2}{4\omega_S^2}-\frac{m_F\dot{\omega}_F^2k_I^2}{4\omega_F^2\kappa_F^2}+\frac{m_S\ddot{\omega}_S}{2\omega_S}, \tag{54}$$

$$\gamma_F=\kappa_F-\frac{3m_F\dot{\omega}_F^2}{4\omega_F^2}+\frac{m_F\ddot{\omega}_F}{2\omega_F}. \tag{55}$$

Therefore, CBOD simplifies the engineering of STA in the system by driving the slow and fast sub-systems independently. In addition, it succeeds in doing so without the need to tailor the interaction term between the two-sub-systems. This is contrary to the exact CD, which involves a controlled modulation in time of all the potential terms in the original Hamiltonian, including the interaction.

As CBOD relies on the BOA, the dynamics generated by the Hamiltonian (53) is not strictly adiabatic. The exact solution to the corresponding time-independent Schrödinger equation can be obtained in a similar manner to that shown for the exact solution in the appendix, with a separation into two independent normal-mode harmonic oscillators. The nonadiabatic evolution of each normal-mode harmonic oscillator can then be described exactly by a self-similar transformation of the corresponding wave function Φ at the start of the evolution. For a harmonic oscillator of mass m and frequency $\omega(t)$ the scaling symmetry determines the evolution of the ground state according to [1, 23, 89, 90]

$$\Phi(t)=\frac{1}{\sqrt{b(t)}}\exp\left(\mathrm{i}\frac{m\dot{b}(t)}{2\hbar b(t)}x^2-\mathrm{i}\frac{\omega_0}{2}\int_0^t\mathrm{d}t'\frac{1}{b(t')^2}\right)\Phi\left(\frac{x}{b(t)};\,0\right), \tag{56}$$

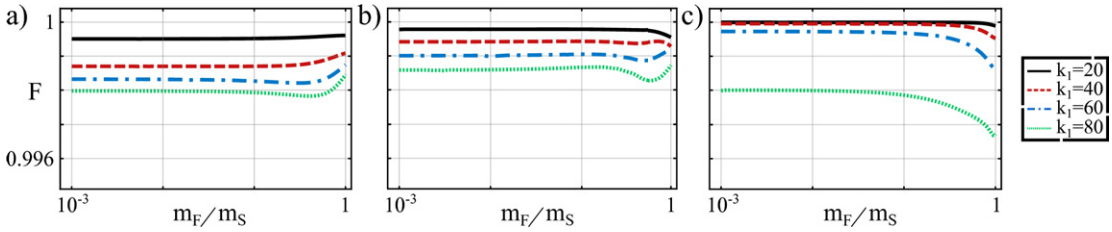

Figure 2. Fidelity under counterdiabatic Born–Oppenheimer dynamics (CBOD). The ramping of a single spring constant of two coupled harmonic oscillators is considered, according to the time modulation in equation (58). Under exact CD, a system initialized in the ground state evolves into the ground state of the final Hamiltonian upon completion of the ramp. CBOD approximates the required controls to assist adiabaticity, facilitating their implementation. The fidelity between the final state evolved under the exact CD and CBOD is shown (for $t = T_f = 1$) in three different cases, corresponding to the modulation of one of each of the spring constants in the systems Hamiltonian: (a) ramping κ_S, with $k_I = 50$, $\kappa_F = 100$, $k_0 = 50$. (b) Ramping κ_F, with $k_I = 50$, $\kappa_S = 100$, $k_0 = 50$. (c) Ramping k_I, with $\kappa_S = \kappa_F = 100$, $k_0 = 1$.

where $\omega_0 = \omega(0)$ and $b(t) > 0$ is a scaling factor obtained by solving the Ermakov equation

$$\ddot{b}(t) + \omega(t)^2 b(t)^2 = \frac{\omega_0^2}{b(t)^3}, \tag{57}$$

with boundary conditions $b(0) = 1$ and $\dot{b}(0) = 0$. By solving the above Ermakov equation numerically for the parameters of Hamiltonian (53), the exact evolution of the system under CBOD can be obtained via equation (56).

5.3. CBOD validity

To investigate the validity of the CBOD technique we consider the following modulation of the spring constant

$$K(t) = k_0 + \frac{k_1}{T_f}\left[t - \frac{T_f}{2\pi}\sin\left(\frac{2\pi}{T_f}t\right)\right], \tag{58}$$

where k_0 and k_1 are offset and strength parameters of the ramping, respectively, and T_f is the time-scale of the modulation, with a single modulation after $t = T_f$. This ramp has first and second derivatives that vanish at $t = 0$ and T_f, favoring adiabatic evolution [91], e.g., over a linear ramp. We will consider a ramping of the individual terms in Hamiltonian (36), i.e. κ_S, κ_F and k_I.

We show the fidelity of the ground state under a ramping of each spring constant in figure 2, i.e.

$$F = |\langle \Psi_{\text{Exact}}(T_f)|\Psi_{\text{CBOD}}(T_f)\rangle|^2. \tag{59}$$

From the assessment of the validity of the BOA in this example, see figure 1, the CBOD technique is expected to be particularly sensitive to ramping the interaction spring constant. A significant drop off in fidelity is observed as the interaction strength is increased by the ramp. Overall, CBOD matches with high fidelity the exact adiabatic evolution. This is reflected by the values $F \geqslant 0.99$ observed in figure 2.

For large ramps of the interaction spring constant, the dotted green lines of figure 2, a slight breakdown of the validity of CBOD for $m_F/m_S \sim 1$ becomes manifest. This is most likely due to the momentum approximation of equation (50), which was required to decouple the fast momentum and slow coordinates in the CD control terms within the BOA. This approximation is only valid in the limit of $m_F/m_S \ll 1$ and/or $k_I \ll \kappa_F$, which are both broken in this scenario. Hence, the lower fidelity of the CBOD protocol for large mass ratio. The breakdown of the CBOD for $m_F/m_S \sim 1$ is consistent with the breakdown of the BOA. Provided that the fast and slow degrees of freedom can so be defined, CBOD can generate high fidelity evolution of states under fast modulations.

However, by contrast to exact CD, CBOD is not valid for arbitrarily fast modulations. CBOD trades the possibility of engineering arbitrarily fast STA for the ability to treat interacting systems which may not be exactly solvable and to simplify the experimental implementation of the required control terms in these systems. The behavior of CBOD under faster modulations is investigated in figure 3, by the fidelity of the exact and CBOD techniques at the end of the process $t = T_f$. As would be expected, the fidelity decreases with faster ramping times, T_f but the fidelity remains high ($F \geqslant 0.9$) and this trend continues for smaller T_f, for which the fidelity exhibits a plateau. In figure 3, each ramp is of a moderate strength and as this strength is increased the fidelity decreases, as was shown in figure 2. Therefore, despite the dependence of the fidelity on the modulation time, CBOD can be used for fast driving of the system.

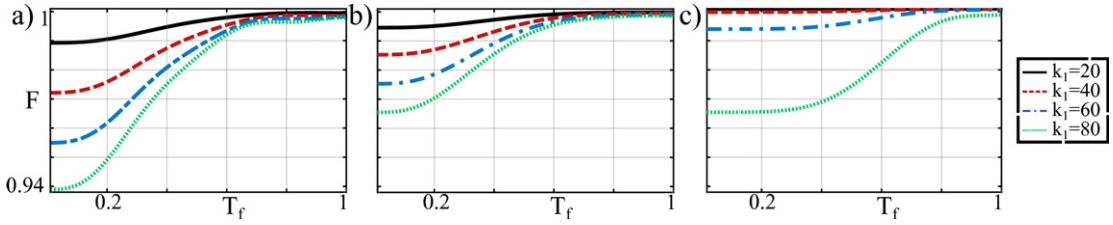

Figure 3. Speed of counterdiabatic Born–Oppenheimer dynamics (CBOD). The ramping of a single spring constant of two coupled harmonic oscillators is considered as a function of the ramping time T_f, according to the time modulation in equation (58). The fidelity between the final state evolved under the exact CD and CBOD is shown in three different cases (for $t = T_f$), corresponding to the modulation of one of each of the spring constants in the systems Hamiltonian: (a) ramping κ_S, with $k_I = 50, \kappa_F = 100, k_0 = 50$. (b) Ramping κ_F, with $k_I = 50, \kappa_S = 100, k_0 = 50$. (c) Ramping k_I, with $\kappa_S = \kappa_F = 100, k_0 = 1$.

6. CBOD in trapped charged particles

CBOD can be used to design of STA in systems that are not exactly solvable, or more generally, easily tractable, analytically or numerically. To demonstrate this, we consider two particles interacting via a Coulomb potential, with the slow particle being confined by a harmonic trap and the fast particle feeling only an attractive Coulomb-like interaction. This model is similar to that of Hooke's atom, which is exactly solvable for certain parameter values. The model Hamiltonian is

$$\hat{H} = \frac{\hat{\mathbf{p}}_S^2}{2m_S} + \frac{\hat{\mathbf{p}}_F^2}{2m_F} + \frac{1}{2}m_S\omega_S^2\hat{r}_S^2 - \frac{g}{|\hat{r}_F - \hat{r}_S|}, \tag{60}$$

where g is an interaction strength and $\hat{r}$ is the radial coordinate of the spherical coordinate system for each of the slow and fast particles. To justify a separation of variables under BOA, we assume that $m_S \gg m_F$. In this section, we will derive the form of the CBOD drivings for this model.

Under the BOA, the slow and fast Hamiltonian are

$$\hat{H}_S = \frac{\hat{\mathbf{p}}_S^2}{2m_S} + \frac{1}{2}m_S\omega_S^2\hat{r}_S^2 + \varepsilon(\hat{r}_S), \tag{61}$$

$$\hat{H}_F = \frac{\hat{\mathbf{p}}_F^2}{2m_F} - \frac{g}{|\hat{r}_F - \hat{r}_S|}. \tag{62}$$

The fast sub-system has the form of the hydrogen atom Hamiltonian which has known solutions,

$$|\psi_F(r_F', \theta, \phi)\rangle = |R_{n,l}(r_F')\rangle \otimes |Y_{l,m}(\theta, \phi)\rangle, \tag{63}$$

where $\hat{r}_F' = \hat{r}_F - \hat{r}_S$. The solutions to the radial $|R_{n,l}(r_F')\rangle$ and angular $|Y_{l,m}(\theta, \phi)\rangle$ separation of this wave function can be found by solving the separated Schrödinger equations, see [63, 84, 92], and are characterized by three quantum numbers (n, l, m). The corresponding eigenvalues depend only on the principal quantum number n and take the form

$$\varepsilon = -\frac{m_F g^2}{2\hbar^2 n^2}. \tag{64}$$

The reduced Hamiltonian thus becomes

$$\hat{H}_S = \frac{\hat{\mathbf{p}}_S^2}{2m_S} + \frac{1}{2}m_S\omega_S^2\hat{r}_S^2 - \frac{m_F g^2}{2\hbar^2 n^2}, \tag{65}$$

which has harmonic oscillator solutions with energy

$$E_{u,n} = \hbar\omega_S\left(u + \frac{3}{2}\right) - \frac{m_F g^2}{2\hbar^2 n^2}. \tag{66}$$

We consider the driving of the system by modulating the interaction strength $g = g(t)$. Under the BOA the dynamics arises only in the fast sub-system, as the slow sub-systems state is invariant under a driving of g. The g-dependence of the fast sub-system state is entirely contained within the radial component of the wave function [84, 92, 93], which takes the normalised form

$$|R_{n,l}(r_F')\rangle = \left(\frac{2m_F g}{\hbar^2 n}\right)^{\frac{3}{2}}\sqrt{\frac{(n-l-1)!}{2n(n+l)!}}\exp\left(-\frac{m_F g r_F'}{\hbar^2 n}\right)\left(\frac{2m_F g r_F'}{\hbar^2 n}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2m_F g r_F'}{\hbar^2 n}\right), \tag{67}$$

where $L_m^{\alpha}(x)$ are the generalised Laguerre polynomials. In this scenario, it is helpful to write the CD term as

$$\hat{H}_{1,F}(t) = \mathrm{i}\hbar\sum_{n,l}(\dot{g}|\partial_g R_{n,l}\rangle\langle R_{n,l}| - \dot{g}\langle R_{n,l}|\partial_g R_{n,l}\rangle|R_{n,l}\rangle\langle R_{n,l}|). \tag{68}$$

We obtain the g derivative of the radial component as

$$\dot{g}|\partial_g R_{n,l}(r_F')\rangle = \left[\frac{3}{2} - \frac{m_F g r_F'}{\hbar^2 n} + (n-1) - (n+l)\frac{L_{n-l-2}^{2l+1}\left(\frac{2m_F g r_F'}{\hbar^2 n}\right)}{L_{n-l-1}^{2l+1}\left(\frac{2m_F g r_F'}{\hbar^2 n}\right)}\right]\frac{\dot{g}}{g}|R_{n,l}(r_F')\rangle, \tag{69}$$

where we have simplified the expression using the generalised Laguerre polynomial recurrence relations [94]. The Berry connection, $\dot{g}\langle R_{n,l}|\partial_g R_{n,l}\rangle$, takes the form of a known definite integral [95] and is found to be

$$\dot{g}\langle R_{n,l}|\partial_g R_{n,l}\rangle = \frac{\dot{g}}{g}\left[\frac{1}{2} - \frac{n}{2} - \frac{l(l+1)}{2n} - \frac{2g^2 m_F^2 (n+1)}{\hbar^4 n^3}\frac{\Gamma(2l+2)(1)_{n-l-2}(2l+2)_{n-l-1}}{(n-l-2)!(n+l)!}\right], \tag{70}$$

with $\Gamma(a)$ the gamma function and $(a)_k$ the Pochhammer symbol, i.e. $(a)_k = \Gamma(a+k)/\Gamma(a)$. Using equations (69) and (70) it is possible to construct the CBOD fast CDs in general. For the sake of illustration, we consider the system to be prepared in the low energy states. We can compactly write the form for the CD of single states for the ground state $(n,l) = (1,0)$

$$H_{F,1} = \mathrm{i}\hbar\left(\frac{3}{2} - \frac{m_F g r_F'}{\hbar^2}\right)\frac{\dot{g}}{g}|R_{1,0}\rangle\langle R_{1,0}|, \tag{71}$$

which is an energy term plus a potential linear in the radial coordinate. The first excited state is degenerate with $(n,l) = (2,0)$ or $(n,l) = (2,1)$, and each has a different CD term, for $(2,0)$

$$H_{F,1} = \mathrm{i}\hbar\left(3 - \frac{g m_F (g m_F + \hbar^2 r_F')}{2\hbar^4} - \frac{2\hbar^2}{\hbar^2 - g m_F r_F'}\right)\frac{\dot{g}}{g}|R_{2,0}\rangle\langle R_{2,0}|, \tag{72}$$

and for $(2,1)$

$$H_{F,1} = \mathrm{i}\hbar\left(\frac{7}{2} - \frac{m_F g r_F'}{2\hbar^2}\right)\frac{\dot{g}}{g}|R_{2,1}\rangle\langle R_{2,1}|. \tag{73}$$

We see that for higher energy states, the form of the CD, equation (68), required can be more complex, with $1/r_F'$ potentials for the $(2,0)$ state, as the CD has a term proportional to the ratio of two Laguerre polynomials from the derivative equation (69).

This example illustrates how CBOD can prove useful to engineer STA in complex systems. In this particular model, the full Hamiltonian is not easily solvable. Yet, the derivation of the CBOD auxiliary controls is made possible by relating the sub-system Hamiltonians to well-known solvable models. More generally, we expect that CBOD helps cracking the complexity barrier in the design of STA by harnessing the separation of energy scales between different degrees of freedom, whenever present.

7. Conclusions

STA provide control protocols to guide the dynamics of quantum and classical systems along an adiabatic reference trajectory, without relying on slow driving. A universal approach to designing STA is provided by the CD technique that guides the evolution of an arbitrary quantum system by means of auxiliary control fields. However, determining the auxiliary controls requires knowledge of the spectral properties of the system, hindering its application to complex systems.

In this work, we have introduced CBOD as a framework to design STA in complex systems. CBOD identifies the required controls to speed up the dynamics of the system by invoking the BOA whenever a separation between fast and slow degrees of freedom is justified. In such a scenario, the required CD terms for the fast and slow variables can be obtained in two-subsequent steps, which in the spirit of the BOA, avoids the need to diagonalize the high-dimensional Hamiltonian of the full system. Thus, CBOD facilitates the finding of the required Hamiltonian controls to speed up the dynamics, in scenarios where spectral properties are not readily available. In addition, CBOD also simplifies the implementation of the STA by reducing the need to control the coupling between fast and slow degrees of freedom. We have demonstrated the validity of CBOD by testing it in a paradigmatic test-bed of the BOA, an exactly-solvable model of two driven coupled harmonic oscillators with unequal masses for which CBOD competes with the exact CD in the preparation of a target state. We have also applied CBOD to the design of STA in a more complex Coulomb system. We anticipate that the CBOD

technique should facilitate the fast nonadiabatic control of the dynamics of complex systems in the plethora of scenarios in which the BOA has proved useful.

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Appendix. Two coupled harmonic oscillators with unequal masses

A.1. Exact solution

The exact solution to the Schrödinger equation of Hamiltonian (37) is well-known [80]. First, we transform the position and momentum spaces canonically via the transformations

$$\begin{pmatrix}\hat{p}_1\\ \hat{p}_2\end{pmatrix}=\begin{pmatrix}(m_F/m_S)^{\frac{1}{4}} & 0\\ 0 & (m_S/m_F)^{\frac{1}{4}}\end{pmatrix}\begin{pmatrix}\hat{p}_S\\ \hat{p}_F\end{pmatrix}, \tag{A1}$$

and

$$\begin{pmatrix}\hat{x}_1\\ \hat{x}_2\end{pmatrix}=\begin{pmatrix}(m_S/m_F)^{\frac{1}{4}} & 0\\ 0 & (m_F/m_S)^{\frac{1}{4}}\end{pmatrix}\begin{pmatrix}\hat{x}_S\\ \hat{x}_F\end{pmatrix}. \tag{A2}$$

This is followed by a rotation of the coordinates

$$\begin{pmatrix}\hat{y}_1\\ \hat{y}_2\end{pmatrix}=\begin{pmatrix}\cos\alpha & -\sin\alpha\\ \sin\alpha & \cos\alpha\end{pmatrix}\begin{pmatrix}\hat{x}_1\\ \hat{x}_2\end{pmatrix}, \tag{A3}$$

under which the momentum is invariant. To diagonalize the system the rotation angle is found to be

$$\alpha(t)=\frac{1}{2}\arctan\left(\frac{2k_I(t)}{\kappa_S(t)\sqrt{\frac{m_F}{m_S}}-\kappa_F(t)\sqrt{\frac{m_S}{m_F}}}\right). \tag{A4}$$

The Hamiltonian is then diagonalized into normal modes, i.e., two independent harmonic oscillators

$$\hat{H}_0(t)=\frac{\hat{p}_1^2}{2\mu}+\frac{\hat{p}_2^2}{2\mu}+\frac{1}{2}\kappa_1(t)\hat{y}_1^2+\frac{1}{2}\kappa_2(t)\hat{y}_2^2, \tag{A5}$$

with reduced mass $\mu=\sqrt{m_S m_F}$ and spring constants

$$\kappa_1(t)=\sqrt{\frac{m_F}{m_S}}\kappa_S(t)\cos^2\alpha+\sqrt{\frac{m_S}{m_F}}\kappa_F(t)\sin^2\alpha+2k_I(t)\sin\alpha\cos\alpha, \tag{A6}$$

$$\kappa_2(t)=\sqrt{\frac{m_F}{m_S}}\kappa_S(t)\sin^2\alpha+\sqrt{\frac{m_S}{m_F}}\kappa_F(t)\cos^2\alpha-2k_I(t)\sin\alpha\cos\alpha. \tag{A7}$$

The solution to the time-independent Schrödinger equation of Hamiltonian (A5) is that of two independent harmonic oscillators in the coordinates y_1 and y_2 with total energy

$$\epsilon_{ij}(t)=\hbar\omega_1(t)\left(i+\frac{1}{2}\right)+\hbar\omega_2(t)\left(j+\frac{1}{2}\right), \tag{A8}$$

with $i,j=0,1,2,\ldots$ and frequencies $\omega_{1,2}(t)=\sqrt{\kappa_{1,2}(t)/\mu}$. The full wave functions take the form of the usual Harmonic oscillator solutions, i.e.

$$\psi_{ij}(y_1,y_2)=\frac{1}{\sqrt{2^{i+j}i!j!}}\left(\frac{\mu^2\omega_1\omega_2}{(\pi\hbar)^2}\right)^{\frac{1}{4}}\exp\left(-\frac{\mu}{2\hbar}(\omega_1 y_1^2+\omega_2 y_2^2)\right)H_i\left(\sqrt{\frac{\mu\omega_1}{\hbar}}y_1\right)H_j\left(\sqrt{\frac{\mu\omega_2}{\hbar}}y_2\right). \tag{A9}$$

With the exact driving utilised in the main text the time-evolution will be the adiabatic solution

$$\psi_{ij}(y_1,y_2,t)=\exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\epsilon_{ij}(t')\right)\psi_{ij}(y_1,y_2). \tag{A10}$$

A.2. BOA for two coupled harmonic oscillators

We now consider Hamiltonian (37) in the regime of $m_S \gg m_F$, where the BOA is valid. Following the steps of section 2.1, the time-independent Schrödinger equation of the fast sub-system reads

$$\left[\frac{\hat{p}_T^2}{2m_F} + \frac{1}{2}\kappa_S'(t)x_S^2 + \frac{1}{2}\kappa_F(t)\hat{x}_T^2\right]\phi_n(x_F;\, x_S) = \varepsilon_n(x_S)\phi_n(x_F;\, x_S), \tag{A11}$$

with transformed coordinate $\hat{x}_T = \left(\hat{x}_F - \frac{k_I(t)}{\kappa_F(t)}x_S\right)$, momentum $\hat{p}_T = \hat{p}_F$ and slow sub-system spring constant $\kappa_S'(t) = \kappa_S(t) - \frac{k_I(t)^2}{\kappa_F(t)}$. Equation (A11) has solutions of a harmonic oscillator in the x_T coordinate,

$$\phi_n(x_T) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m_F\omega_F}{\pi\hbar}\right)^{\frac{1}{4}}\exp\left(-\frac{m_F}{2\hbar}\omega_F x_T^2\right)H_n\left(\sqrt{\frac{m_F\omega_F}{\hbar}}x_T\right), \tag{A12}$$

with eigenvalues

$$\varepsilon_n(x_S) = \hbar\omega_F(t)\left(n + \frac{1}{2}\right) + \frac{1}{2}\kappa_S'(t)x_S^2, \tag{A13}$$

and frequency $\omega_F(t) = \sqrt{\kappa_F(t)/m_F}$.

The slow sub-system then follows the Schrödinger equation of

$$\left[\frac{\hat{p}_S^2}{2m_S} + \hbar\omega_F(t)\left(n + \frac{1}{2}\right) + \frac{1}{2}\kappa_S'(t)\hat{x}_S^2\right]\psi(x_S) = E\psi(x_S), \tag{A14}$$

which will have harmonic solutions in x_S

$$\psi_\nu(x_S) = \frac{1}{\sqrt{2^\nu \nu!}}\left(\frac{m_S\omega_S}{\pi\hbar}\right)^{\frac{1}{4}}\exp\left(-\frac{m_S}{2\hbar}\omega_S x_S^2\right)H_\nu\left(\sqrt{\frac{m_S\omega_S}{\hbar}}x_S\right) \tag{A15}$$

with frequency $\omega_S = \sqrt{\kappa_S'(t)/m_S}$. Note, that $\kappa_S'(t)$ can be negative, turning the frequency imaginary and the solutions considered in this work incorrect. We will take care to ensure that we remain in the real frequency limit, i.e. $\kappa_S(t)\kappa_F(t) > k_I(t)^2$. The total energy of the system will be

$$E_{n,\nu} = \hbar\omega_S(t)\left(\nu + \frac{1}{2}\right) + \hbar\omega_F(t)\left(n + \frac{1}{2}\right), \tag{A16}$$

and total wave function for a single modes is

$$\Psi_{n\nu} = \phi_n\psi_\nu. \tag{A17}$$

A.3. Relaxed BOA

We next consider the application of the relaxed BOA to the coupled harmonic oscillators. The Berry connection in equation (12) and geometric tensor given by equation (13) are both integrals of the fast (or reduced) sub-system wave functions, ϕ_n, which are given in equation (A12). In particular, we consider the fast sub-system to be in the ground state,

$$\phi_0 = \left(\frac{m_F\omega_F}{\pi\hbar}\right)^{\frac{1}{4}}\exp\left(-\frac{m_F\omega_F}{2\hbar}x_T^2\right). \tag{A18}$$

The Berry connection identically vanishes

$$\mathcal{A}_0 = \mathrm{i}\langle\phi_0|\partial_{x_S}\phi_0\rangle = 0, \tag{A19}$$

and the geometric tensor simply reads

$$g_0 = \langle\partial_{x_S}\phi_0|\partial_{x_S}\phi_0\rangle = \frac{k_I(t)^2\omega_F(t)m_F}{2\hbar\kappa_F(t)^2}. \tag{A20}$$

Excited states of the fast sub-system also result in a vanishing Berry connection and a geometric tensor of similar form to above. Therefore within the relaxed BOA, the coupled oscillator problem has the same wave functions as the conventional BOA but with a different total energy. That difference is the value of the geometric tensor multiplied by a factor, as shown in equation (11). In this example, the relaxed and conventional CDs are identical, as the wave functions coincide.

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